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CHEMICAL CHALLENGE PROGRAMSubmission of
Additional Robust Summaries for**ISODECYL/PHENYL PHOSPHITE CATEGORY:**

| Chemical Name <i>(synonym)</i> | Abbreviation | CAS No. |
|--|---------------------|----------------|
| Phosphorous acid, triisodecyl ester <i>(triisodecyl phosphite)</i> | TDP | 25448-25-3 |
| Phosphorous acid, diisodecyl phenyl ester <i>(diisodecylphenyl phosphite)</i> | PDDP | 25550-98-5 |
| Phosphorous acid, isodecyl diphenyl ester <i>(isodecyldiphenyl phosphite)</i> | DPDP | 26544-23-0 |
| Phosphorous acid, triphenyl ester <i>(triphenyl phosphite)</i> | TPPi | 101-02-0 |

PHOSPHITE MANUFACTURERS CONSORTIUM (PMC)1250 Connecticut Avenue, NW, Suite 700,
Washington, DC 20036
Phone: (202) 419-1500

November 15, 2006

PHYSICAL/CHEMICALS ELEMENTS

MELTING POINT

Test Substance

Identity: TDP
Remarks: Test substance source: Dover Chemical Corp., #162T041801
Purity: > 99% (MSDS)

Method

Method: OECD Guideline 102 (OECD, 1993)
GLP: Yes
Year: 2002
Test Conditions: The melting point was determined by recording the warming curve (temperature vs. time) of a frozen test sample, and also by recording visual observations during the melting process. The method was calibrated using deionized water. The thermocouple calibration data showed an average absolute bias of less than 0.2 °C. Thermocouple temperatures were not adjusted for this insignificant bias. The report indicates that there were no deviations from protocol.

Results

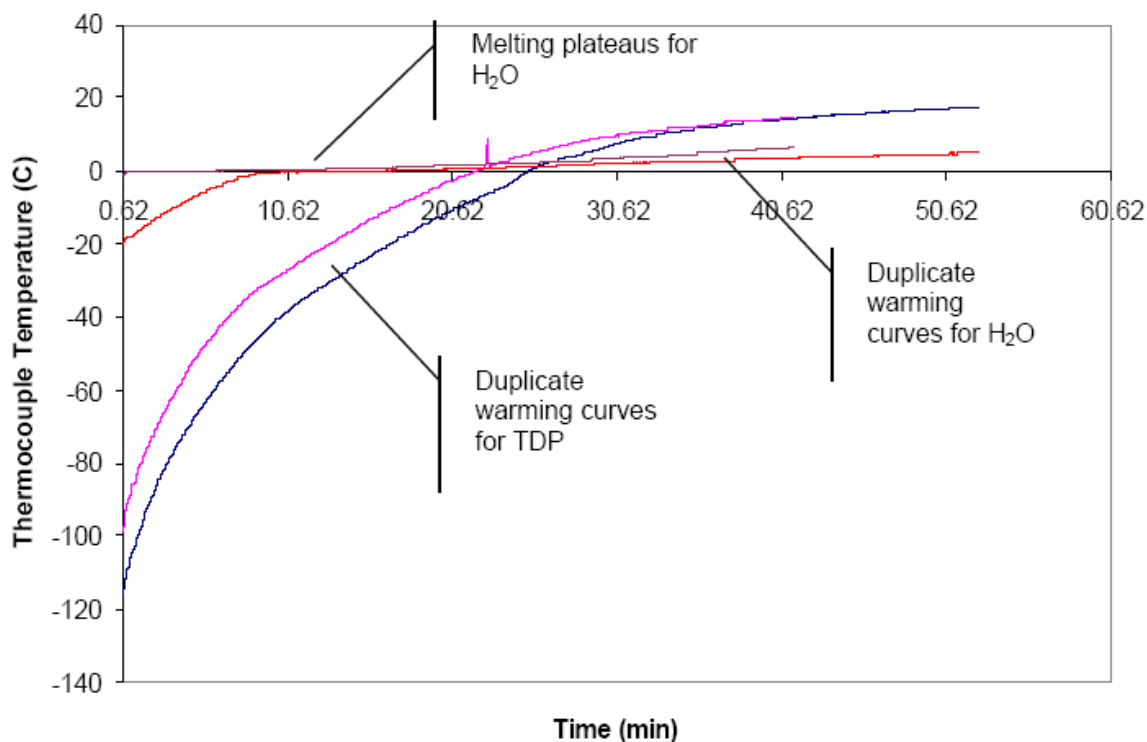
Melting point: -91 to -64 °C
Decomposition: No
Sublimation: No
Remarks: The warming curve for deionized water (approximately 20 mL) showed the expected plateau at 0 °C indicating acceptable method calibration. When frozen TDP (approximately 20 mL) was warmed, the melting of TDP was first observed at approximately -91 °C and the entire TDP sample was observed to have melted at approximately -64 °C.

Visual Melting Observations on TDP

| Observation | Thermocouple Temperature (°C) | | Average | SD | % RSD |
|-----------------------|-------------------------------|-------------|---------|----|-------|
| | Replicate 1 | Replicate 2 | | | |
| First sign of melting | -88 | -94 | -91 | 3 | 3 |
| Melting Completed | -58 | -70 | -64 | 6 | 9 |

Phosphorous acid, triisodecyl ester (TDP), CAS No. 25448-25-3

Warming curves for TDP and Deionized Water



Conclusions

The average melting point of TDP was -91 to -64 °C. Unlike water, the TDP warming curve did not contain plateaus at the melting point, indicating that the melting of TDP was essentially non-endothermic.

Reliability

Klimisch code: 1

Remarks: This report represents data generated in accordance with the following Good Laboratory Practice Standards. OECD ENV/MC/CHEM(98)17, Paris, Jan. 26, 1998. All phases of this study were conducted according to the above GLPs.
(Author)

Reference

Reimer, G. "Physical/Chemical Property of Triisodecyl Phosphite (TDP), CAS # 25448-25-3 - Melting Point (OECD 102)." Study No. 10301 1312. Report to General Electric Company, Reimer Analytical & Associates Inc., Vancouver, BC. February 24, 2002.

BOILING POINT (THERMAL DEGRADATION)

Test Substance

Identity: TDP
Remarks: Tradename: Doverphos 6; Source Dover Chemical Company.
Sample lot no. 162T041801.
Purity: > 99% (MSDS)

Method

Method: OECD Guideline 103 (OECD, 1993)
GLP: Yes
Year: 2002
Test Conditions: Test was done in duplicate. Note TDP is sensitive to moisture. TDP (~ 25 mL) was placed in a clean dry round bottom flask (~50 mL) fitted with a clean water condenser and a calibrated thermometer. The thermometer bulb was above the TDP. Boiling chips were added and the flask contents were heated to reflux. The temperature of the reflux vapors was measured every minute until 4 readings were within 1°C. Using clean apparatus and the same thermometer, the boiling point of deionized water was similarly measured in duplicate. Ambient air pressure during the experiment was 100.0 kPa (750.1 mm Hg).

Results

Boiling point: 187 ± 3 °C
Pressure: 100.1 kPa
Decomposition: No
Remarks: The method bias for the boiling point of water was 2 °C. The observed duplicate boiling points of TDP were 191 °C and 186 °C for an average of 189 ± 3 °C. The bias corrected boiling point was 187 ± 3 °C at 100.1 kPa (750.1 mm Hg)

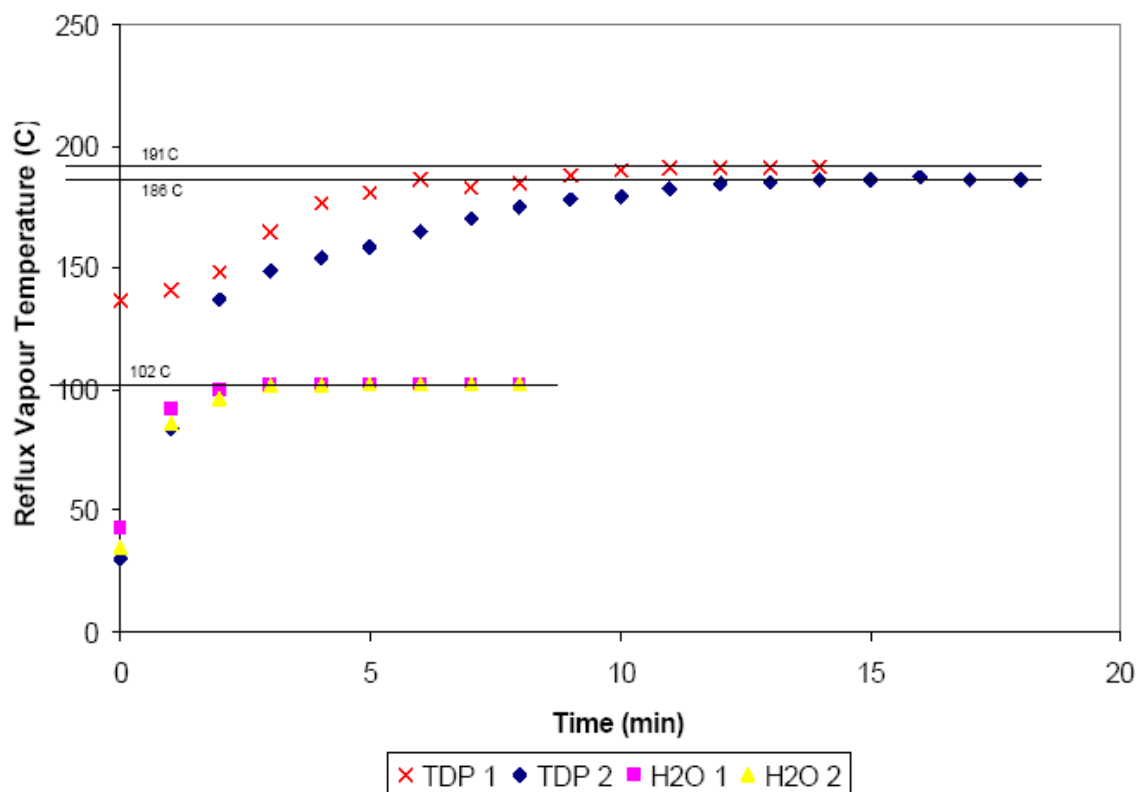


Figure 1. Reflux vapour temperatures.

Conclusions

Boiling point of TDP is 187 ± 3 °C at 100.1 kPa

Reliability

Klimisch Code: 1

Remarks: This report represents data generated in accordance with the following Good Laboratory Practice Standards. OECD ENV/MC/CHEM(98)17, Paris, Jan. 26, 1998. All phases of this study were conducted according to the above GLPs.
(Author)

Reference

Reimer, G. "Physical/Chemical Property of Triisodecyl Phosphite (TDP), CAS # 25448-25-3 - Boiling Point (OECD 103)." Study No. 10301 1312. Report to General Electric Company. Reimer Analytical & Associates Inc., Vancouver, BC. February 1, 2002.

VAPOR PRESSURE

Test Substance

Identity: TDP

Method

Method: Calculated with ACD model

GLP: No

Year: 2002

Test Conditions: Vapor pressure test was not conducted since the calculated vapor pressure was determined to be three orders of magnitude lower than the detection limit of the most sensitive (gas saturation) method (1x 10⁻⁵ Pa, OECD Guideline 104, 1993).

Vapor pressure calculation was performed using computer software manufactured by Advanced Chemistry Development Inc., Toronto Ontario. This software uses the following calculation method proposed by Hass and Newton in the CRC Handbook on Chemistry and Physics.”

$$\Delta_{vap}H(T_b) = \left[(\varphi \cdot 2.303 \cdot R \cdot T_b(K)) \right] \cdot 0.839594 + 3.9039$$

Results

Vapor Pressure: 2.18 x 10⁻⁸ Pa at 25 °C

Conclusions

The calculated vapor pressure of TDP is 2.18 x 10⁻⁸ Pa at 25 °C.

Reliability

Klimisch Code: 2

References

Reimer, G. “Physical/Chemical Property of Triisodecyl Phosphite (TDP), CAS # 25448-25-3 - Vapor Pressure (OECD 104) - Expert Statement.” Study No. 10301 1312. Report to General Electric Company. Reimer Analytical & Associates Inc., Vancouver, BC. August 28, 2002.

Phosphorous acid, triisodecyl ester (TDP), CAS No. 25448-25-3

Advanced Chemistry Development Inc. ACD Vapor Pressure Calculation
Software Toronto, Ontario, Canada, 2001.

PARTITION COEFFICIENT

Test Substance

Identity: TDP

Method

Method: Calculated using ACD Pow software model.
GLP: No
Year: 2002
Test Conditions: It was not possible to perform the n-octanol/water partition coefficient (Pow) test on triisodecyl phosphite (TDP) because of its hydrolysis during the test procedure. The n-octanol/water partition coefficient (Pow) was calculated using computer software manufactured by ACD Toronto, Canada. Comparison of ACD calculated Pow values with experimentally observed values for several different classes of organic compounds showed correlations generally greater than 0.9 indicating that the ACD calculation method is generally valid for the estimation of Pow.

Results

Pow: 12.9
Temperature: 25 °C

Conclusions

The calculated Pow of triisodecyl phosphite (TDP) was 12.9 (25 °C) and i-decanol, the final organic hydrolysis product of TDP, was 3.9 (25 °C).

Reliability

Klimisch Code: 2

References

Reimer, G. "Physical/Chemical Property of Triisodecyl Phosphite (TDP), CAS # 25448-25-3 - n-Octanol/Water Partition Coefficient (OECD 107) - Expert Statement." Study No. 10301 1312. Report to General Electric Company. Reimer Analytical & Associates Inc., Vancouver, BC. August 28, 2002.

Advanced Chemistry Development Inc. ACD Pow Calculation Model Toronto
Ontario, 2002

WATER SOLUBILITY

Test Substance

Identity: TDP

Method

Method: Calculated with ACD model
GLP: No
Year: 2003
Test Conditions: It was not possible to perform the water solubility test on triisodecyl phosphite (TDP) because of its hydrolysis during the test procedure. Water solubility was calculated using computer software manufactured by ACD. Comparison of ACD-calculated water solubilities with experimentally observed values, for several different classes of organic compounds showed correlations generally greater than 0.9 indicating that the ACD calculation method is generally valid for the estimation of water solubility. (Author)

Results

Value: 1×10^{-1} g/L at 25 °C

Conclusions

The calculated water solubility of TDP is 1×10^{-1} g/L at 25 °C. The water solubilities of the final TDP hydrolysis products i-decanol and phosphorous acid are 0.18 g/L at 25 °C (calculated) and 87 weight percent at 40 °C respectively (CRC, 1974) (Author)

Reliability

Klimisch Code: 2

References

Reimer, G. "Physical/Chemical Property of Triisodecyl Phosphite (TDP), CAS # 25448-25-3 - Water Solubility (OECD 105) - Expert Statement." Study No. 10301 1312. Report to General Electric Company. Reimer Analytical & Associates Inc., Vancouver, BC. July 21, 2003.

Phosphorous acid, triisodecyl ester (TDP), CAS No. 25448-25-3

Advanced Chemistry Development Inc. ACD Aqueous Solubility v6.0 Calculation
Model Toronto Ontario, 2002

CRC (1974) Handbook of Chemistry and Physics, CRC Press, 55th ed.

ENVIRONMENTAL FATE AND PATHWAYS ELEMENTS

PHOTODEGRADATION

Test Substance

Identity: TDP

Method

Method: EPIWIN(v3.10)\AopWin v.1.90
Type: hydroxyl radical reaction
GLP: No
Year: 2004
Test Conditions: Atmospheric oxidation estimated using
EPIWIN(v3.10)\AopWin v.1.90 Hydroxyl radical reaction.
Assumes 12 hour day, 1.5×10^6 OH/cm³

Results / Conclusion

Temperature: 25 °C
Half-life $t_{1/2}$: 0.103 days (1.231 hours)
Rate Constant: 104.2496×10^{-12} cm³/molecule-sec

Reliability

Klimisch Code: 2

Reference

Report on Triisodecyl Phosphite (TDP, CAS No. 25448-25-3) Generated Using
EPIWIN(v3.10)\AopWin v. 1.90. June 2004.

STABILITY IN WATER

Test Substance

Identity: TDP

Method

| | |
|------------------------|---|
| Method: | OECD 111 |
| Test type: | Hydrolytic stability |
| GLP: | Yes |
| Year: | 2002 |
| Test Conditions: | Study plan deviated from OECD 111 in that it contained the limitation that TDP must be sufficiently soluble in test buffers to be detected by the analytical method. This limitation was found to be applicable as TDP aqueous solubility was insufficient. Therefore the study plan protocol could not be executed. Experiments were performed to investigate the hydrolysis of TDP in which acetonitrile cosolvent (up to 50%) was employed to facilitate dissolution of TDP. |
| Duration: | 17 hours |
| Negative Controls: | Deionized water |
| Analytical procedures: | HPLC |

Results

Two experiments were performed in which aqueous buffer/CH₃CN (1:1, V:V) solutions at pH 5, pH 7, pH9 of TDP analyzed via HPLC over a period of approximately 17 hours. The concentrations of TDP in these solutions decreased with time and the concentrations of the i-decanol hydrolysis product increased with time in the four reactions, due to TDP hydrolysis. These TDP hydrolysis reactions followed first-order kinetics. The observed half-lives for TDP in aqueous solutions, each with 50% CH₃CN cosolvent, at pH 5, pH 7, pH 9 and deionized water are listed in the table below.

Observed Aquatic Half-Lives of TDP, Each with 50% CH₃CN cosolvent, 23 ± 1 °C

| Parameter | pH 5 | pH 7 | pH 9 | DIW |
|-----------------------------|------|-----------------|-------|--------|
| Average Rate Constant (1/h) | 0.17 | 0.03 | 0.035 | 0.0446 |
| SD | 0.03 | 0.01 | 0.001 | 0.0002 |
| RSD | 19% | 42% | 4% | 0.4% |
| Average Half-life (h) | 4.1 | 17 ⁷ | 20.1 | 15.53 |
| SD | 0.8 | 1 ⁸ | 0.8 | 0.07 |
| RSD | 19% | | 4% | 0.4% |

⁷ this value was eliminated as an outlier, based on the results at pH 9 and in deionized water, and also on a report that organophosphites are stabilized by base (Stevenson, Don R. Phosphite stabilizers; new developments. AddCon Asia '97, Int. Plast. Addit. Modif. Conf. (1997), paper10/1-paper10/7 Publisher: Rapra Technology, Shrewsbury, UK.).

⁸ estimated based on values for other reactions

Conclusion

Experimental results indicated that, due to the low water solubility of TDP, a relatively sensitive extraction method would be required to analyze test solutions generated in an OECD hydrolysis test. It was also observed that TDP hydrolyzed fairly rapidly at 23 C in aqueous/acetonitrile (1/1) solutions, with half-lives ranging from 4 to 20 hours over a pH range of 5 to 9 respectively. Results also suggested that these half-lives would decrease in the absence of cosolvent. Therefore it was concluded that the OECD hydrolysis test, which requires the use of < 1% organic solvent, could not be conducted because of interference caused by the hydrolysis of TDP during analyses of the test solutions. (Author)

Reliability

Klimisch Code: 1 (Reliable without restriction)
Remarks: This report represents data generated in accordance with the following Good Laboratory Practice Standards. OECD ENV/MC/CHEM(98)17, Paris, January 26, 1998. All phases of this study were conducted according to the above standards.

Reference

Reimer, G. "Physical/Chemical Property of Triisodecyl Phosphite (TDP), CAS # 25448-25-3 - Hydrolytic Stability (OECD 111)." Study No. 10301 1312. Report to General Electric Company. Reimer Analytical & Associates Inc., Vancouver, BC. July 5, 2002.

TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY)

Test Substance

Identity: TDP

Method

Type: Level III
Remarks: EPIWIN v 3.10

Phosphorous acid, triisodecyl ester (TDP), CAS No. 25448-25-3

Results/Conclusion

| | Mass Amount (%) | Half-Life (Hrs) | Emissions (kg/hr) |
|----------|-----------------|--------------------|-------------------|
| Air | 0.0406 | 2.46 | 1000 |
| Water | 2.37 | 1.44×10^3 | 1000 |
| Soil | 29.2 | 1.44×10^3 | 1000 |
| Sediment | 68.4 | 5.76×10^3 | 0 |

Reliability

Klimisch Code: 2

References

Report on Triisodecyl Phosphite (TDP, CAS No. 25448-25-3) Generated Using EPIWIN(v3.10)\AopWin v. 1.90. June 2004.

BIODEGRADATION

Test Substance

Identity: TDP
Remarks: Doverphos 6
Purity: > 99%

Method

Method: OECD 301D Closed Bottle Test and
BC Research Standard Operating Procedure (SOP 1706)
Type: Aerobic
Year: 2003
Contact time: 28 days
Inoculum: Secondary effluent from Lulu Island Domestic Wastewater
Treatment Plant, Richmond, BC
Test Conditions: The biodegradability was assessed by measuring the
biological oxygen demand (BOD) of a microbial population
(secondary effluent) exposed to low concentrations of the test
substance under controlled conditions, and by comparing that
BOD to the theoretical oxygen demand (ThOD) of the test
substance.
The test incubation temperature stated in the study plan was
 20 ± 1 °C; however, the incubation temperature ranged from
18 to 24 °C during the study. A study plan deviation for this
change is included in Appendix A of the study document.

A series of five test solutions were used in the test: inoculum blank control, filter paper control, test substance treatment, reference substance treatment and toxicity control.

The reference substance employed in this study was sodium benzoate, CAS 535-32-1, which is classified as readily biodegradable. It was used as a positive control to assess test validity. The toxicity control bottles contained both test and reference substances and was used to determine if the test substance inhibited inoculum metabolism.

Secondary effluent from Lulu Island Domestic Wastewater Treatment Plant, Richmond, BC was used as a source of inoculum in the test, rather than Polyseed (as proposed on the study plan) since it was not considered to be an acceptable source of inoculum by the regulatory authorities that were consulted. A study plan amendment for this change was included in Appendix A of the study document.

Test substance was weighed onto filter paper before addition to the test vessels. Both the filter paper and the test substance were added to the test vessels. Test vessels were inverted several times every day to promote mixing of the test solution.

BOD and percent degradation was calculated according to OECD Guidelines 301D.

Cumulative degradation was plotted versus time, using Excel 97 SR2 (Microsoft 1997) to visually assess the rates at which the test substance and the reference substance were degrading.

Significant differences in mean DO concentrations between the two controls (inoculum blank and filter paper blank) and percent degradation between the reference substances treatment and toxicity control were assessed with the Wilcoxon paired sample test according to the methods described in Zar (1984)

Confirmation of the concentration of test substance in the test solutions was not conducted because the test substance was expected to hydrolyze during the analytical procedure.

Percent degradation for the test substance, reference substance and toxicity control were calculated using nominal concentrations.

Results

The test substance did not degrade by 10%; therefore, a 10-day window could not be applied to assess ready biodegradability. The highest percentage degradation

was observed on day 10 when it was 2.62%. On day 28, 1.31% of the test substance was degraded. A lag phase and degradation phase for the test substance did not occur.

Mean Biological Oxygen Demand (mg O₂/mg chemical)

| Day | Test Substance | Reference Substance | Toxicity Control |
|------------|-----------------------|----------------------------|-------------------------|
| 3 | 0.01 | N/A | N/A |
| 7 | 0.04 | 1.41 | 1.49 |
| 10 | 0.01 | N/A | N/A |
| 14 | -0.02 | 1.44 | 1.32 |
| 16 | 0.08 | N/A | N/A |
| 18 | 0.04 | N/A | N/A |
| 21 | -0.01 | 1.44 | 1.58 |
| 24 | -0.02 | N/A | N/A |
| 28 | 0.04 | 1.37 | 1.70 |

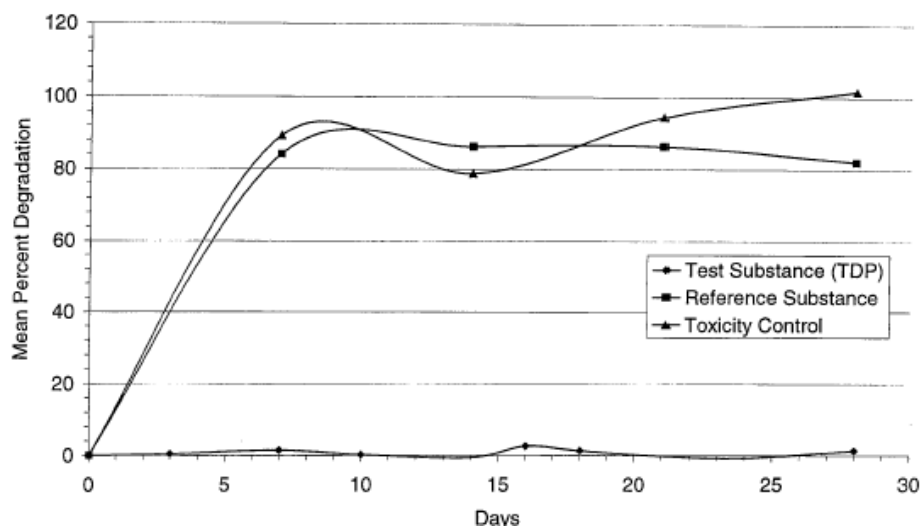
Mean Percent Degradation (%)

| Day | Test Substance | Reference Substance | Toxicity Control |
|------------|-----------------------|----------------------------|-------------------------|
| 3 | 0.47 | N/A | N/A |
| 7 | 1.43 | 84.1 | 89.2 |
| 10 | 0.21 | N/A | N/A |
| 14 | -0.53 | 86.2 | 78.7 |
| 16 | 2.62 | N/A | N/A |
| 18 | 1.36 | N/A | N/A |
| 21 | -0.17 | 86.4 | 94.5 |
| 24 | -0.67 | N/A | N/A |
| 28 | 1.31 | 82.0 | 102 |

There was no significant difference in percent biodegradation between the reference substance treatment and the toxicity control (Wilcoxon paired-sample test, $p > 0.05$)

The test was considered valid based on the test validity criteria.

**Figure: Degradation of Test Substance (TDP),
Reference Substance and Toxicity Control**



The results of this study indicated that the test substance and its hydrolysis products were not readily biodegradable. Percent degradation did not reach > 60% in a 10 day window within the 28 day test period, and only reached 1.31% by the end of the test. The test substance was non-inhibitory, based on 102% biodegradation of the toxicity control (containing test substance and reference substance) as compared to the 82% biodegradation of the reference substance alone.

Conclusions

The test substance TDP was not readily biodegradable when tested according to OECD 301D. (Author)

Reliability

Klimisch Code: 1

Remarks: This report represents data generated in accordance with the following Good Laboratory Practices (GLP) Standards: OECD Principles of Good Laboratory Practice (OECD, 1998). All phases of this study were conducted according to the above GLP standards.

Reference

Kinnee, K. "Closed Bottle Test of Triisodecyl Phosphite (CAS No. 25448-25-3) Using OECD Guidelines 301D (TOX2002)." BCR Study ID: TOX2002. Report to General Electric Company. BC Research Inc., Vancouver, BC. May 28, 2003.

ECOTOXICITY ELEMENTS

CONSOLIDATED ACUTE TOXICITY TO FISH, TOXICITY TO AQUATIC PLANTS, ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity: TDP

Method

In attempting to design appropriate studies to investigate the acute ecotoxicity of TDP in algae, daphnids and fish, it was discovered that the testing would be difficult to conduct in compliance with OECD Guidance Document #23 entitled “Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures” (OECD 2000) because of the inherent physical/chemical properties of the test substance (i.e., extremely poor water solubility and rapid hydrolysis at the calculated limit of solubility). On this basis, the US EPA was consulted to ascertain how best to approach the ecotoxicological testing of this test substance. Through these consultations, it was concluded that, since direct measurements of the ecotoxicity of the parent test substance would likely be very difficult the testing program should focus on quantifying the toxicity of the combination of hydrolysis by-products of ‘aged’ TDP.

Measured and calculated aquatic toxicity values (EC_{50}) for the individual primary hydrolysis by-products of TDP (isodecanol and phosphorous acid) were identified. With these data, estimates of the acute ecotoxicity values (solution toxicity values) based on the sum of the ratios of the maximum theoretical concentration of the individual hydrolysis by-products (i.e., “aged” TDP) in solution (at the limit of solubility) and their representative ecotoxicity values (EC_{50}) were found to be 3.6×10^{-8} (algae), 1.4×10^{-8} (daphnids) and 2.8×10^{-8} (fish). Since a derived solution toxicity value of 1.0 is considered to be equivalent to an EC_{50} for the “aged” solutions, the further below a value is from 1 the lower the inferred ecotoxicity hazard. On this basis, these findings indicate that the mixture of hydrolysis by-products arising from a standard solution of TDP would not be toxic to aquatic organisms.

It is possible to quantitatively predict the maximum theoretical concentration of hydrolysis by-products and resulting toxicity of the solution of these by-product based on the known toxicity of the individual by-products, assuming additive toxicity.

On this basis, a detailed literature search was conducted to assess the available database of information pertaining to the acute toxicity of isodecanol and

phosphorous acid to fish (rainbow trout), daphnids and algae. Where sufficient data were unavailable in the scientific literature, ECOSAR (US EPA 2001) was used to model the potential ecotoxicity of the hydrolysis by-products of TDP. A summary of the acute ecotoxicity data for these byproducts to these organisms is provided in the report.

By this method, a solution toxicity value of 1.0 is considered equivalent to an acute EC₅₀ value (*i.e.*, it would predict 50% acute mortality /growth inhibition in the test species, based on the theoretical concentrations).

Results

Based on the following stoichiometry:

One mole TDP (molecular weight = 502.79 g/mole) yields three moles isodecanol (molecular weight = 158.29 g/mole) and one mole phosphorous acid (molecular weight = 82.00 g/mole);

At its aqueous solubility limit of 0.1 ng/L (or less), TDP would hydrolyse to 5.4×10^{-13} moles/L isodecanol and 1.8×10^{-13} moles/L phosphorous acid. These molar concentrations equate to mass concentrations of 8.6×10^{-8} mg isodecanol/L and 1.5×10^{-8} mg phosphorous acid/L, respectively. The modeling of the solution toxicity values for the mixture of hydrolysis by-products of TDP at its aqueous solubility limit in fish, daphnids, and algae are summarized below.

| Aquatic Toxicity Values | Isodecanol EC ₅₀ (mg/L) | Calculated Isodecanol Solution Concentration (mg/L) | Phosphorous Acid EC ₅₀ (mg/L) ^c | Calculated Phosphorous Acid Solution Concentration (mg/L) | Calculated Solution Toxicity Value |
|-------------------------|------------------------------------|---|---|---|------------------------------------|
| Fish | 3.1 ^m | 8.6×10^{-8} | 383 | 1.5×10^{-8} | 2.8×10^{-8} |
| Daphnids | 6.2 ^m | 8.6×10^{-8} | 387 | 1.5×10^{-8} | 1.4×10^{-8} |
| Algae | 2.4 ^c | 8.6×10^{-8} | 230 | 1.5×10^{-8} | 3.6×10^{-8} |

^m = measured value (derived from toxicity database, scientific literature).

^c = calculated value (using ECOSAR; US EPA, 2001).

Conclusions

The predicted solution toxicity values attributable to the mixture of TDP hydrolysis by-products were calculated to be 3.6×10^{-8} (algae), 1.4×10^{-8} (daphnids) and 2.8×10^{-8} (fish). These values are well below 1.0 indicating that the mixture of hydrolysis by-products arising from a saturated solution of TDP would essentially be not toxic to aquatic organisms. (Author)

Reliability

Klimisch Code: 2

References

GlobalTox International Consultants Inc., Guelph ON. "Consolidated Report - Alternative to Ecotoxicity Testing - Modeling the Potential Toxicity to Aquatic Organisms - Hydrolysis By-Products of Triisodecyl Phosphite (CASRN 25448-25-3.)" Report to General Electric Company. July 17, 2003.

HEALTH ELEMENTS

COMBINED REPEAT DOSE/REPRODUCTIVE/DEVELOPMENTAL TOXICITY

Test Substance

| | |
|-----------|-------------------------------|
| Identity: | TDP |
| Remarks: | Doverphos 6, Batch 162T041801 |
| Purity: | > 99% |

Method

| | |
|--|-------------------------------|
| Method: | OECD 422 (modified) |
| Type: | 2 generation |
| GLP: | Yes |
| Year: | 2005 |
| Species: | rat |
| Strain: | Sprague-Dawley |
| Route of administration: | gavage |
| Doses/concentration levels: | 0, 50, 250 and 1000 mg/kg/day |
| Sex: | Male and Female |
| Control group and treatment: | Yes, once per day |
| Frequency of treatment: | once per day |
| Duration of test: | 8 weeks |
| Premating exposure period for males (P and F1) as appropriate: | 2 weeks |
| Premating exposure period for females (P and F1) as appropriate: | 2 weeks |

The purpose of this study was to evaluate the potential of TDP administered by oral gavage once daily, 7 days per week in CD rats to cause toxic characteristics from repeated dosing, encompassing 2-week prebreed, mating (for both sexes), gestation, and lactation (for F0 females). This study also evaluated the potential of

TDP to cause possible effects on parental male and female reproductive performance (such as gonadal function, mating behavior, conception, development of the conceptus, parturition) and offspring survival, growth, and development through lactation and weaning. This study was performed in compliance with OECD Guideline 422, (1996) and was performed under OECD (1998), and EPA TSCA (1989) Good Laboratory Practice regulations. This study exceeded the OECD 422 study design by following the F1 offspring to weaning.

Male and female CD (Sprague-Dawley(SD)) F0 rats were administered TDP orally by gavage at 0, 50, 250 and 1000 mg/kg/day at a dose volume of 5 ml/kg/day in Mazola[®] corn oil, 10 animals/sex/dose, for 2 weeks of prebreed exposure (males and females), 2 weeks of mating (males and females) and 3 weeks of gestation and lactation each (F0 females). Body weights and feed consumption for the F0 males and females were recorded weekly during the prebreed period for both sexes and for F0 females during gestation and lactation. Clinical signs were recorded at least once daily for F0 males and females until necropsy. Functional Observational Battery (FOB) including home cage observations, handling observations, open field observations, sensory and neuromuscular observations and physiological observations, was performed on all initial animals once during quarantine and at least once per week for F0 animals during prebreed, mating (both sexes), gestation and lactation (F0 females). After the 2-week prebreed exposure period, animals were randomly mated within treatment groups for a 2-week mating period to produce the F1 generation, with continuing exposure.

Five F0 males and five F0 females per dose group were evaluated for auditory function, motor activity, and assessment of grip strength prior to necropsy. All F0 parental animals were necropsied with complete histologic evaluation of 5 selected males and females in the 0 and 1000 mg/kg/day groups.

On the day of birth (postnatal day [pnd] 0), anogenital distance was measured and body weights recorded for all live F1 pups in all litters. F1 litters were culled on pnd 4 to yield as nearly as possible 5 males and 5 females per litter. The culled F1 pups were weighed, euthanized, and necropsied with complete external and visceral examinations. For the remaining F1 pups, survival indices were calculated at least weekly through weaning (pnd 21). In addition, hematology, clinical biochemistry and urinalysis assays were performed at necropsy for 5 randomly selected F0 males. Clinical biochemistry was also assessed for the 28-day females.

Results

TDP administered by gavage once daily at 0, 50, 250 and 1000 mg/kg/day to parental F0 CD (SD) rats, 10/sex/group through prebreed, mating, gestation and lactation resulted in essentially no treatment- or dose-related adult F0 parental toxicity at any dose at any time. Reproductive toxicity was not present in F0

males and females. There was also no F1 offspring toxicity observed postnatally through the weanling necropsy. Therefore, the F0 male and female systemic no observable adverse effect level (NOAEL) was at or above 1000 mg/kg/day. The NOAELs for F0 reproductive toxicity during lactation were also at or above 1000 mg/kg/day for males and females.

Conclusions

TDP administered by gavage once daily at 0, 50, 250 and 1000 mg/kg/day to parental F0 CD (SD) rats, 10/sex/group through prebreed, mating, gestation and F1 lactation resulted in essentially no treatment or dose related adult F0 parental toxicity at any dose at any time. Reproductive toxicity was not present in F0 males or females. There was also no F1 offspring toxicity observed postnatally through the weanling necropsy. Therefore, the F0 male and female systemic no observable adverse effect level (NOAEL) was at or above 1000mg/kg/day for males and females. The NOAELs for F0 reproductive toxicity were observed at or above 1000 mg/kg/day for males and females. The NOAELs for F1 offspring toxicity during lactation were also at or above 1000 mg/kg/day for males and females. (Author)

Reliability

| | |
|----------------|--|
| Klimisch Code: | 1 (Reliable without restriction) |
| Remarks: | This study was conducted in compliance with the OECD (1998) and EPA TSCA (1989) Good Laboratory Practices Guidance. (Author) |

Reference

Tyl, RW, Myers, CB and Marr, MC. "Modified Combined Repeated Dose Toxicity Study with the Reproductive/Developmental Toxicity Screening Test of Triisodecyl Phosphite (TDP) Administered Via Oral Gavage to CD® (Sprague-Dawley) Rats (OECD 422)." RTI Identification No. 65C-09178.000.500. Report to Phosphite Manufacturers Consortium, RTI International, Research Triangle Park, NC. April 26, 2005.

PHYSICAL/CHEMICALS ELEMENTS

MELTING POINT

Test Substance

Identity: PDDP

Method

Method: EPIWIN (MPBPWIN v. 1.40)

GLP: No

Year: 2004

Results

Melting point: 90.17 °C

Conclusions

The melting point value was calculated as 90.17 °C using EPIWIN (MPBPWIN v. 1.40).

Reliability

Klimisch Code: 2

References

Report on Diisodecylphenyl Phosphite (PDDP, CAS No. 25550-98-5) Generated Using EPIWIN (MPBPWIN v. 1.40). 2004.

BOILING POINT (THERMAL DEGRADATION)

Test Substance

Identity: PDDP

Method

Method: EPIWIN (MPBPWIN v. 1.40) Adapted Stein and Brown Method

GLP: No

Year: 2004

Phosphorous acid, diisodecyl phenyl ester (PDDP), CAS No. 25550-98-5

Results/Conclusion

Boiling point: 478.99 °C

Reliability

Klimisch Code: 2

References

Report on Diisodecylphenyl Phosphite (PDDP, CAS No. 25550-98-5) Generated Using EPIWIN (MPBPWIN v. 1.40). 2004.

VAPOR PRESSURE

Test Substance

Identity: PDDP

Method

Method: EPIWIN (MPBPWIN v 1.40), 2004 (Modified grain method)
GLP: No
Year: 2004
Test Conditions: Model

Results

Vapor Pressure: 2.19×10^{-8} mm Hg at 25 °C

Conclusions

Vapor Pressure value was calculated to be 2.19×10^{-8} mm Hg at 25 °C using EPIWIN (MPBPWIN v 1.40)

Reliability

Klimisch Code: 2

References

Report on Diisodecylphenyl Phosphite (PDDP, CAS No. 25550-98-5) Generated Using EPIWIN (MPBPWIN v. 1.40). 2004.

PARTITION COEFFICIENT

Test Substance

Identity: PDDP

Method

Method: EPIWIN (KOWWIN v 1.66)
GLP: No
Year: 2004
Test Conditions: It was not possible to perform the n-octanol/water partition coefficient (Pow) test on Phosphorous acid, diisodecyl phenyl ester (PDDP) because of its hydrolysis during the test procedure. The n-octanol/water partition coefficient (Pow) was calculated using EPIWIN (KOWWIN v 1.66).

Results

Log Kow: 9.32
Temperature: 25 °C

The log octanol-water partition coefficient (SRC) was calculated to be 9.32 using KOWWIN v. 1.66.

Conclusions

The log octanol-water partition coefficient (SRC) was calculated to be 9.32 using KOWWIN v. 1.66.

Reliability

Klimisch Code: 2

References

Report on Diisodecylphenyl Phosphite (PDDP, CAS No. 25550-98-5) Generated Using EPIWIN (KOWWIN v. 1.66). 2004.

WATER SOLUBILITY

Test Substance

Identity: PDDP

Method

Method: WSKOW v. 1.40
GLP: No
Year: 2004
Test Conditions: It was not possible to perform the water solubility test on Phosphorous acid, diisodecyl phenyl ester (PDDP) because of its hydrolysis during the test procedure. Water solubility was calculated using EPIWIN v3.10 (WSKOW v 1.40). Estimate log Kow of 9.32 was used. No melting point equation used.

Results

Value: 1.914×10^{-5} mg/L at 25 °C

Conclusions

See results

Reliability

Klimisch Code: 2

References

Report on Diisodecylphenyl Phosphite (PDDP, CAS No. 25550-98-5) Generated Using EPIWIN (KOWWIN v. 1.66). 2004.

ENVIRONMENTAL FATE AND PATHWAYS ELEMENTS

PHOTODEGRADATION

Test Substance

Identity: PDDP

Method

Method: EPIWIN(v3.10)\AopWin v. 1.90
Type: hydroxyl radical reaction
GLP: No
Year: 2004

Phosphorous acid, diisodecyl phenyl ester (PDDP), CAS No. 25550-98-5

Test Conditions: Atmospheric oxidation estimated using
EPIWIN(v3.10)\AopWin v. 1.90 Hydroxyl radical reaction.
Assumes 12 hour day, 1.5×10^6 OH/cm³

Results/Conclusion

Temperature: 25 °C
Half-life t_{1/2}: 0.150 days (1.796 hours)
Rate Constant: 71.4496×10^{-12} cm³/molecule-sec

Reliability

Klimisch Code: 2

References

Report on Diisodecylphenyl Phosphite (PDDP, CAS No. 25550-98-5) Generated
Using EPIWIN(v3.10)\AopWin v. 1.90. June 2004.

STABILITY IN WATER

Test Substance

Identity: PDDP

Method

Method: EPIWIN3.10 (HYDROWIN v. 1.67)
Tset type: Hydrolytic stability
GLP: No
Year: 2004
Test Conditions: Model to calculate aqueous base/acid catalyzed hydrolysis at
25 °C

Results/Conclusion

Rate constants can NOT be calculated for this structure (HYDROWIN v. 1.67)

Reliability

Klimisch Code: 2

Phosphorous acid, diisodecyl phenyl ester (PDDP), CAS No. 25550-98-5

References

Report on Diisodecylphenyl Phosphite (PDDP, CAS No. 25550-98-5) Generated Using EPIWIN v. 3.10 (HYDROWIN v1.67). 2004.

TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY)

Test Substance

Identity: PDDP

Method

Type: Level III
Remarks: EPIWIN v 3.10

Results/Conclusion

| | Mass Amount (%) | Half-Life (Hrs) | Emissions (kg/hr) |
|----------|-----------------|-------------------|-------------------|
| Air | 0.0875 | 3.59 | 1000 |
| Water | 3.4 | 900 | 1000 |
| Soil | 28.9 | 900 | 1000 |
| Sediment | 67.6 | 3.6×10^3 | 0 |

Reliability

Klimisch Code: 2

References

Report on Diisodecylphenyl Phosphite (PDDP, CAS No. 25550-98-5) Generated Using EPIWIN v. 3.10. May 2004.

PHYSICAL/CHEMICAL ELEMENTS

MELTING POINT

Test Substance

Identity: DPDP

Method

Method: EPIWIN (MPBPWIN v. 1.40)

GLP: No

Year: 2004

Results

Melting point: 154.75 °C

Conclusions

Melting point was calculated to be 154.75 °C (EPIWIN).

Reliability

Klimisch Code: 2

References

Report on Isodecyldiphenyl Phosphite (DPDP, CAS No. 26544-23-0) Generated Using EPIWIN (MPBPWin v. 1.40). 2004.

BOILING POINT (THERMAL DEGRADATION)

Test Substance

Identity: DPDP

Method

Method: EPIWIN (MPBPWIN v. 1.40) Adapted Stein and Brown Method

GLP: No

Year: 2004

Phosphorous acid, isodecyl diphenyl ester (DPDP), CAS No. 26544-23-0

Results

Boiling point: 435.74 °C

Conclusions

Remarks: Boiling point is 435.74 °C

Reliability

Klimisch Code: 2

References

Report on Isodecyldiphenyl Phosphite (DPDP, CAS No. 26544-23-0) Generated Using EPIWIN (MPBPWin v. 1.40). 2004.

VAPOR PRESSURE

Test Substance

Identity: DPDP

Method

Method: EPIWIN (MPBPWIN v 1.40), 2004 ((Modified grain method)
GLP: No
Year: 2004
Test Conditions: Model

Results

Vapor Pressure: $5.2 \cdot 10^{-8}$ mm Hg at 25 °C

Conclusions

Vapor Pressure value was calculated to be $5.2 \cdot 10^{-8}$ mm Hg at 25 °C using EPIWIN (MPBPWIN v 1.40)

Reliability

Klimisch Code: 2

References

Report on Isodecyldiphenyl Phosphite (DPDP, CAS No. 26544-23-0) Generated Using EPIWIN (MPBPWin v. 1.40). 2004.

PARTITION COEFFICIENT

Test Substance

Identity: DPDP

Method

Method: EPIWIN v 3.10 (KOWWIN v1.66)

GLP: No

Year: 2004

Test Conditions: It was not possible to perform the n-octanol/water partition coefficient test on Phosphorous acid, isodecyl diphenyl ester (DPDP) because of its hydrolysis during the test procedure. The n-octanol/water partition coefficient was calculated using EPIWIN v 3.10 (KOWWIN v1.66)

Results

Log Kow: 8.52

Temperature: 25 °C

Conclusions

The n-octanol/water partition coefficient of Phosphorous acid, isodecyl diphenyl ester (DPDP) was calculated using EPIWIN v 3.10 (KOWWIN v1.66) to be log Kow = 8.52.

Reliability

Klimisch Code: 2

References

Report on Isodecyldiphenyl Phosphite (DPDP, CAS No. 26544-23-0) Generated Using EPIWIN v 3.10 (KOWWIN v. 1.66). May 2004.

WATER SOLUBILITY

Phosphorous acid, isodecyl diphenyl ester (DPDP), CAS No. 26544-23-0

Test Substance

Identity: DPDP

Method

Method: WSKOW v1.40
GLP: No
Year: 2004
Test Conditions: It was not possible to perform the water solubility test on Phosphorous acid, isodecyl diphenyl ester (DPDP) CAS No 26544-23-0 because of its hydrolysis during the test procedure. Water solubility was calculated using EPIWIN v3.10 (WSKOW v 1.40). Estimate log Kow of 8.52 was used. No melting point equation used.

Results/Conclusion

Value: 2.331×10^{-4} mg/L at 25 °C

Reliability

Klimisch Code: 2

References

Report on Isodecyldiphenyl Phosphite (DPDP, CAS No. 26544-23-0) Generated Using EPIWIN v 3.10 (KOWWIN v. 1.66). May 2004.

ENVIRONMENTAL FATE AND PATHWAYS

PHOTODEGRADATION

Test Substance

Identity: DPDP

Method

Method: EPIWIN(v3.10)\AopWin v.1.90
Type: hydroxyl radical reaction
GLP: No
Year: 2004

Phosphorous acid, isodecyl diphenyl ester (DPDP), CAS No. 26544-23-0

Test Conditions: Atmospheric oxidation estimated using
EPIWIN(v3.10)\AopWin v.1.90 Hydroxyl radical reaction.
Assumes 12 hour day, 1.5×10^6 OH/cm³

Results/Conclusion

Temperature: 25 °C
Half-life t_{1/2}: 0.250 days (3.058 hours)
Rate Constant: 41.9781×10^{-12} cm³/molecule-sec

Reliability

Klimisch Code: 2

References

Report on Isodecyldiphenyl Phosphite (DPDP, CAS No. 26544-23-0) Generated
Using EPIWIN v 3.10\AopWin v. 1.90. June 2004.

STABILITY IN WATER

Test Substance

Identity: DPDP

Method

Method: EPIWIN3.10 (HYDROWIN v1.67)
Test type: Hydrolytic stability
GLP: No
Year: 2004
Test Conditions: Model to calculate aqueous base/acid catalyzed hydrolysis at
25 °C

Results/Conclusion

Rate constants can NOT be calculated for this structure (HYDROWIN v 1.67)

Reliability

Klimisch Code: 2

Phosphorous acid, isodecyl diphenyl ester (DPDP), CAS No. 26544-23-0

References

Report on Isodecyldiphenyl Phosphite (DPDP, CAS No. 26544-23-0) Generated Using EPIWIN v 3.10 (HYDROWIN v. 1.67). May 2004.

TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY)

Test Substance

Identity: DPDP

Method

Type: Level III
Remarks: EPIWIN v 3.10

Results/Conclusion

| | Mass Amount (%) | Half-Life (Hrs) | Emissions (kg/hr) |
|----------|-----------------|-------------------|-------------------|
| Air | 0.147 | 6.12 | 1000 |
| Water | 3.42 | 900 | 1000 |
| Soil | 28.7 | 900 | 1000 |
| Sediment | 67.7 | 3.6×10^3 | 0 |

Reliability

Klimisch Code: 2

References

Report on Isodecyldiphenyl Phosphite (DPDP, CAS No. 26544-23-0) Generated Using EPIWIN v 3.10. May 2004.

PHYSICAL/CHEMICAL ELEMENTS

MELTING POINT

Test Substance

Identity: TPPi

Method

Method: Expert Statement

GLP: No

Year: 1975

Results/Conclusion

The melting point of Triphenyl phosphite (TPPi) is approximately 25 °C (author). The reported melting point of TPPi on the CRC Handbook of Chemistry and Physics is approximately 25 °C (CRC 1975). This is an approximate melting point because TPPi does not give a sharp melting point due to its physical/chemical characteristics. The CRC reference is recognized by the US EPA as an acceptable source of physical/chemical parameters (US EPA, 1999).

Reliability

Klimisch Code: 2

References

Reimer, G. "Physical/Chemical Property of Triphenyl Phosphite (TPPi), CAS # 101-02-0 - Melting Point (OECD 102) - Expert Statement." Study No. 10301 1527. Report to General Electric Company, Reimer Analytical & Associates Inc., Vancouver, BC. February 24, 2002.

Weast, RC. (ed.). Handbook of Chemistry and Physics. 55th edition. Cleveland: CRC Press Inc., 1975. p. C-429.

US EPA, Determining the Adequacy of Existing Data. 1999.
<http://www.epa.gov/chemrtk/pubs/general/datadfin.htm>

BOILING POINT (THERMAL DEGRADATION)

Test Substance

Identity: TPPi

Method

| | |
|---------|------------------|
| Method: | Expert Statement |
| GLP: | No |
| Year: | 1976 |

Results

| | |
|----------------|--|
| Boiling point: | >300 °C |
| Pressure: | 101 kPa |
| Remarks: | The reported boiling point of TPPi is 360°C (CRC, 1976). This is an adequate boiling point result because CRC is recognized by US EPA as an acceptable reference source (US EPA, 1999). Due to the reporting limit of 300°C the boiling point of TPPi is reported here as greater than 300°C at 101 kPa. |

Conclusions

The boiling point of triphenyl phosphite (TPPi) is greater than 300° C at 101kPa (author)

Reliability

Klimisch code: 2

References

Reimer, G. "Physical/Chemical Property of Triphenyl Phosphite (TPPi), CAS # 101-02-0 - Boiling Point (OECD 103) - Expert Statement." Study No. 10301 1527. Report to General Electric Company, Reimer Analytical & Associates Inc., Vancouver, BC. December 20, 2001.

Weast, RC. (ed.). Handbook of Chemistry and Physics. 57th edition. Cleveland: CRC Press Inc., 1976., p. C-435.

US EPA. Determining the Adequacy of Existing Data. 1999.
<http://www.epa.gov/chemrtk/pubs/general/datadfin.htm>

VAPOR PRESSURE

Test Substance

Identity: TPPi

Method

Method: EPIWIN (MPBPWIN v 1.40), 2004 ((Modified grain method)
GLP: No
Year: 2004
Test Conditions: Model

Results

Vapor Pressure: 7.63×10^{-5} mm Hg at 25 °C

Conclusions

Vapor Pressure value was calculated to be 7.63×10^{-5} mm Hg at 25 °C using EPIWIN (MPBPWIN v 1.40)

Reliability

Klimisch Code: 2

References

Report on Triphenyl Phosphite (TPPi, CAS No. 101-02-0) Generated Using EPIWIN (MPBPWIN v. 1.40). 2004.

PARTITION COEFFICIENT

Test Substance

Identity: TPPi

Method

Method: ACD model
GLP: No
Year: 2002
Test Conditions: It was not possible to perform the n-octanol/water partition coefficient (Pow) test on triphenyl phosphite (TPPi, CAS 101-01-0) because of its hydrolysis during the test procedure. The n-octanol/water partition coefficient (Pow) was calculated using computer software manufactured by ACD Toronto, Canada. Comparison of ACD calculated Pow values with experimentally observed values for several different classes of organic compounds showed correlations generally

Phosphorous acid, triphenyl ester (TPPi), CAS No. 101-02-0

greater than 0.9 indicating that the ACD calculation method is generally valid for the estimation of Pow.

Results

Pow: 2.5×10^7
Temperature: 25 °C

The calculated Pow of TPPI is 2.5×10^7 at 25 °C. The reported Pow of the final organic TPPI hydrolysis product phenol is 31.6 at 25 °C. (Sangster, 1989)

Conclusions

The calculated Pow of triphenyl phosphite (TPPi) was 2.5×10^7 (25 °C). The calculated Pow of phenol, the final organic hydrolysis product of TPPI, was 31.6 (25 °C).

Reliability

Klimisch Code: 2

References

Reimer, G. "Physical/Chemical Property of Triphenyl Phosphite (TPPi), CAS # 101-02-0 - n-Octanol/Water Partition Coefficient (OECD 107) - Expert Statement." Study No. 10301 1527. Report to General Electric Company, Reimer Analytical & Associates Inc., Vancouver, BC. April 16, 2002.

Advanced Chemistry Development Inc. ACD Pow Calculation Model. Toronto Ontario, 2002.

Sangster, J. "Octanol-water partition coefficients of simple organic compounds." J. Phys. Chem. Ref. Data, 18(3) 1111-229. 1989.

WATER SOLUBILITY

Test Substance

Identity: TPPI

Method

Method: ACD Aqueous Solubility v. 5.0
GLP: No
Year: 2002

Phosphorous acid, triphenyl ester (TPPi), CAS No. 101-02-0

Test Conditions: It was not possible to perform the water solubility test on Triphenyl phosphite (TPPi) because of its hydrolysis during the test procedure. Water solubility was calculated using computer software manufactured by ACD. Comparison of ACD-calculated water solubilities with experimentally observed values, for several different classes of organic compounds showed correlations generally greater than 0.9 indicating that the ACD calculation method is generally valid for the estimation of water solubility. (Author)

Results

Value: 0.3 mg/L at 25 °C

Conclusions

The calculated water solubility of TPPi is 0.3 mg/L at 25 °C. The reported water solubilities of the final TPPi hydrolysis products phenol and phosphorous acid are 80 mg/L at 25 °C and 87 weight percent at 40 °C respectively (CRC, 1974) (Author)

Reliability

Klimisch Code: 2

References

Reimer, G. "Physical/Chemical Property of Triphenyl Phosphite (TPPi), CAS # 101-02-0 - Water Solubility (OECD 105) - Expert Statement." Study No. 10301 1527. Report to General Electric Company, Reimer Analytical & Associates Inc., Vancouver, BC. April 16, 2002.

Advanced Chemistry Development Inc. ACD Aqueous Solubility v. 6.0 Calculation Model Toronto, Ontario. 2002.

CRC (1974). Handbook of Chemistry and Physics, CRC Press, 55th ed.

ENVIRONMENTAL FATE AND PATHWAYS ELEMENTS

PHOTODEGRADATION

Test Substance

Identity: TPPi

Phosphorous acid, triphenyl ester (TPPi), CAS No. 101-02-0

Method

Method: EPIWIN (v3.10)\ AopWin v.1.90
Type: hydroxyl radical reaction
GLP: No
Year: 2004
Test Conditions: Atmospheric oxidation estimated using EPIWIN (v3.10)\ AopWin v.1.90 Hydroxyl radical reaction. Assumes 12 hour day, 1.5×10^6 OH/cm³

Results/Conclusion

Temperature: 25 °C
Half-life $t_{1/2}$: 0.987 days (11.838 hours)
Rate Constant: 10.8423×10^{-12} cm³/molecule-sec

Reliability

Klimisch Code: 2

References

Report on Triphenyl Phosphite (TPPi, CAS No. 101-02-0) Generated Using EPIWIN(v3.10)\AopWin v. 1.90. June 2004.

STABILITY IN WATER

Test Substance

Identity: TPPi
Remarks: Doverphos 10
Purity: 99.7%

Method

Method: HPLC
Test type: Hydrolytic stability
GLP: Yes
Year: 2002
Test Conditions: Study plan deviated from OECD 111 because TPPi must be sufficiently soluble in test buffers to be detected by the analytical method.
The HPLC method used in these studies was based on published reports (Baylocq *et al*, 1986; Stevenson *et al*, 1999; Stevenson, 1997; Munteanu *et al* 1985)

Results

The results of experiments on aqueous/cosolvent TPPi solutions indicated that the half-lives of TPPi in deionized water (initially at pH 6-7) and pH9 buffer were approximately 0.5 hour and less than 14 hours respectively at 22 °C.

Summary of TPPi Hydrolysis rates

| Aqueous Solvent | Cosolvent | Temp (°C) | Rate Constant | Half-life (h) ⁹ | Source |
|--|--------------------|-----------|------------------------|----------------------------|-----------------------------------|
| Aq. HCl; pH 1.3 | (¹⁰) | 25 | 1.8E-4 s ⁻¹ | 1.1 | Al-Lohedan <i>et al.</i> , (1991) |
| Deionized H ₂ O; initial pH 6-7 | Methanol (50%) | 22 | na ¹¹ | ~ 0.5 | BCRI # 252 1518 |
| pH 9 buffer | Acetonitrile (50%) | 22 | na | < 14 | BCRI # 172 1403 |

⁹ this is the estimated half-life in the absence of cosolvent

¹⁰ half-life extrapolated to pure water from results on ethanol/water mixtures

¹¹ not available from the data

Conclusions

Al-Lohendan et al (1991) reported a TPPi hydrolysis half life of 1.1 hour in water at pH 1.3 and 25 °C by extrapolation of results on TPPi solutions in ethanol/water.

The results of experiments on aqueous/cosolvent TPPi solutions indicated that the half-lives of TPPi in deionized water (initially at pH 6-7) and pH 9 buffer were approximately 0.5 h and less than 14 h respectively at 22 °C.

Therefore, due to these relatively short half-lives, a rapid method is required for the analysis of TPPi in aqueous solutions. However, the low water solubility of TPPi precludes such “direct injection” methods. This was shown by the injection of near saturated TPPi solutions in 1% CH₃CH/buffers which showed insufficient HPLC responses. Therefore, an extraction method would be required for the analysis of TPPi in aqueous solutions, which is more time consuming and would likely produce erroneous results due to the relatively rapid hydrolysis of TPPi during the extraction procedure.

It follows that performance of the OECD hydrolysis test was considered not to be technically feasible under normal laboratory conditions. Regarding the hydrolytic pathway of TPPi, literature and experimental evidence indicates that TPPi hydrolyzes essentially completely to phenol and phosphorous acid, with little or no accumulation of the possible di and mono ester hydrolysis products.

Phosphorous acid, triphenyl ester (TPPi), CAS No. 101-02-0

Reliability

Klimisch Code: 4 (Not assignable)

This report represents data generated in accordance with the following Good Laboratory Practice Standards. OECD ENV/MC/CHEM(98)17, Paris, January 26, 1998. All phases of this study were conducted according to the above standards. However, nonstandard protocols were utilized due to the rapid hydrolysis of the test substance.

References

Reimer, G. "Physical/Chemical Property of Triphenyl Phosphite (TPPi), CAS # 101-02-0 - Hydrolytic Stability (OECD 111)." Study No. 10301 1527-Hy. Report to General Electric Company, Reimer Analytical & Associates Inc., Vancouver, BC. December 6, 2002.

Al-Lohedan, Hamad A. "Micellar effects upon acid catalyzed hydrolysis of Triphenyl phosphite." Phosphorous, Sulfur, Silicon Relat. Elem: 63 (3-4), 261-71. 1991.

TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY)

Test Substance

Identity: TPPi

Method

Type: Level III
Remarks: EPIWIN v 3.10

Results/Conclusion

| | Mass Amount (%) | Half-Life (Hrs) | Emissions (kg/hr) |
|----------|-----------------|-------------------|-------------------|
| Air | 0.474 | 23.7 | 1000 |
| Water | 4.44 | 900 | 1000 |
| Soil | 30.3 | 900 | 1000 |
| Sediment | 64.8 | 3.6×10^3 | 0 |

Reliability

Klimisch Code: 2

References

Report on Triphenyl Phosphite (TPPi, CAS No. 101-02-0) Generated Using EPIWIN v. 3.10. June 2004.

BIODEGRADATION

Test Substance

| | |
|-----------|--------------|
| Identity: | TPPi |
| Remarks: | Doverphos 10 |
| Purity: | 99.7% |

Method

| | |
|---------------|---|
| Method; | OECD 302D, Closed Bottle Test |
| Test Type: | Aerobic |
| Year: | 2003 |
| Contact time: | 28 days |
| Inoculum: | Secondary effluent from Lulu Island Domestic Wastewater Treatment Plant, Richmond, BC |

A sample of Triphenyl phosphite (TPPi) was tested to assess its degree of ready biodegradability, using the procedure outlined in OECD 301D for the Closed Bottle Test (OECD (1992)). The biodegradability was assessed by measuring the biological oxygen demand (BOD) of a microbial population (secondary effluent) exposed to a low concentration of test substance under controlled conditions and by comparing that BOD to the theoretical oxygen demand (ThOD) of the test substance.

Test Conditions: The test incubation temperature stated in the study plan was 20 ± 1 °C; however, the incubation temperature ranged from 10 to 24 °C during the study. A study plan deviation for this change is included in Appendix A of the study report. The bottles were gently agitated to improve contact of the inoculum with undissolved test substance by inverting them several times once a day during the test.

Secondary effluent was used as a source of inoculum in the test rather than Polyseed, as Polyseed was not considered to be an acceptable source of inoculum by the regulatory authorities that were consulted. A study plan amended for this change is included in Appendix A of the study document. The nominal concentrations of the test and reference substances are listed in the table below.

Nominal Bottle Concentrations at Test Initiation

| Test Series | Inoculum (cells/L) | Test Substance (mg/L) | Reference Substance (mg/L) |
|----------------------|--------------------|-----------------------|----------------------------|
| Inoculum Blank | 9.0×10^4 | 0 | 0 |
| Filter Paper Control | 9.0×10^4 | 0 | 0 |
| Test Substance | 9.0×10^4 | 10 | 0 |
| Reference Substance | 9.0×10^4 | 0 | 2 |
| Toxicity Control | 9.0×10^4 | 10 | 2 |

A series of five test solutions were used in the test: inoculum blank control, filter paper control, test substance treatment, reference substance treatment, and toxicity control. The inoculum blank determined the biological oxygen demand in the absence of either the reference or test substances. The filter paper control was used to monitor the effect of the filter paper on the inoculum, and to provide the blank oxygen uptake values for bottles containing test substance and filter paper. The reference substance sodium benzoate, CAS No. 532-32-1 is classified as readily biodegradable and was used as a positive control to assess test validity. The toxicity control bottles contained both test and reference substances and was used to determine if the test substance inhibited inoculum metabolism.

Cumulative degradation was plotted versus time using Excel 97 SR-2 (Microsoft 1997) to visually assess the rates at which the test substance and the reference substance were degrading. Significant differences in mean DO concentrations between the two controls (inoculum blank and filter paper blank) and percent degradation between the reference substance treatment and toxicity control were assessed with the Wilcoxon paired sample test according to methods described in Zar (1984)

Confirmation of the concentration of test substance in the test solutions was not conducted because the test substance was expected to hydrolyze during the analytical procedure.

Results

The results of this study indicate that the test substance and its hydrolysis products were not readily biodegradable. Percent degradation did not reach > 60% in a 10 day window within the 28 day test period, and only reached 0.1% by the end of the test. The test substance was non-inhibitory, based on a 79.5% biodegradation of the toxicity control (containing test substance and reference substance) as compared to the 82% biodegradation of the reference substance alone.

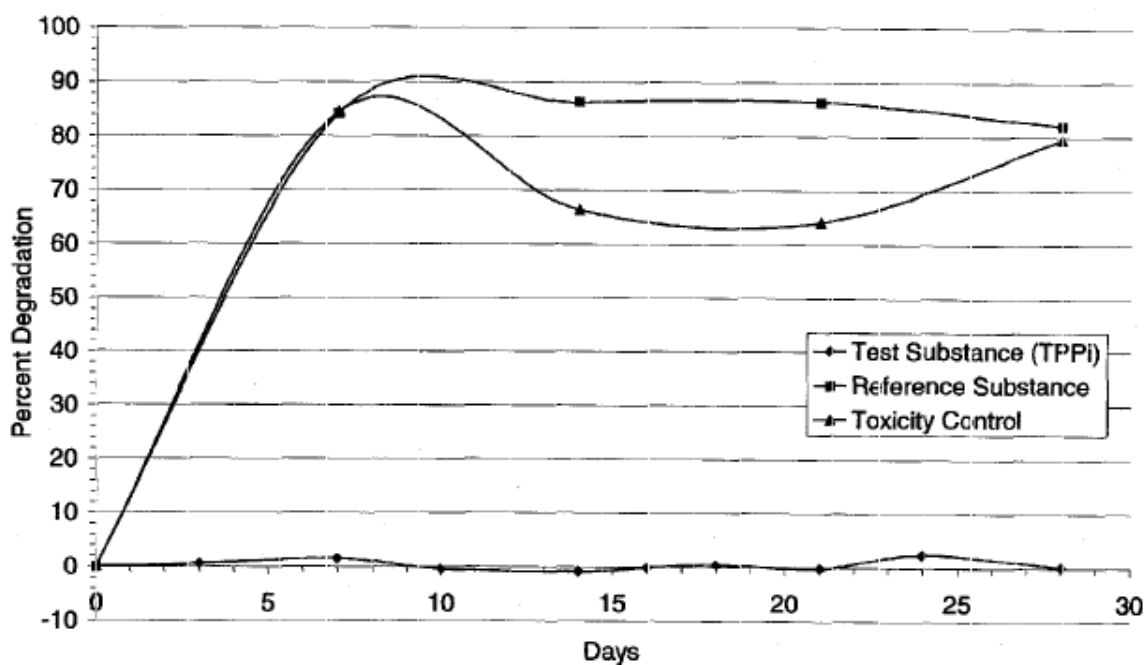
Phosphorous acid, triphenyl ester (TPPi), CAS No. 101-02-0

There was no significant difference in percent biodegradation between the reference substance treatment and the toxicity control (Wilcoxon paired-sample test, $p > 0.05$).

The test was considered valid based on the test validity criteria.

Mean Percent Degradation (%)

| Day | Test Substance | Reference Substance | Toxicity Control |
|-----|----------------|---------------------|------------------|
| 3 | 0.54 | -- | -- |
| 7 | 1.46 | 84.13 | 84.43 |
| 10 | -0.43 | -- | -- |
| 14 | -0.86 | 86.23 | 66.32 |
| 16 | -0.14 | -- | -- |
| 18 | 0.45 | -- | -- |
| 21 | -0.18 | 86.38 | 64.07 |
| 24 | 2.36 | -- | -- |
| 28 | 0.14 | 82.04 | 79.49 |



Conclusion

The test compound TPPi was not readily biodegradable when tested according to OECD 301D.

Reliability

Klimisch Code: 1 (Reliable without restriction)

Remarks: This report represents data generated in accordance with the OECD Guideline for Testing of Chemicals (301D, 1992) and the OECD Principles of Good Laboratory Practice (OECD, 1998) All phases of this study were conducted according to GLP standards. (Author)

References

Serben, K. "Closed Bottle Test of Triphenyl Phosphite (CAS No. 101-02-0) Using OECD Guidelines 301D (TOX1902)." BCR Study ID: TOX1902. Report to General Electric Company. BC Research Inc., Vancouver, BC. July 24, 2003.

ECOTOXICITY ELEMENTS

CONSOLIDATED ACUTE TOXICITY TO FISH, TOXICITY TO AQUATIC PLANTS, ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity: TPPi

Method

In attempting to design appropriate studies to investigate the acute ecotoxicity of TPPi in algae, daphnids and fish, it was discovered that the testing would be difficult to conduct in compliance with OECD Guidance Document #23 entitled "Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures" (OECD 2000) because of the inherent physical/chemical properties of the test substance (i.e., extremely poor water solubility and rapid hydrolysis at the calculated limit of solubility). On this basis, the US EPA was consulted to ascertain how best to approach the ecotoxicological testing of this test substance. Through these consultations, it was concluded that, since direct measurements of the ecotoxicity of the parent test substance would likely be very difficult the testing program should focus on quantifying the toxicity of the combination of hydrolysis by-products of 'aged' TPPi.

Measured and calculated aquatic toxicity values (EC_{50}) for the individual primary hydrolysis by-products of TPPi (phenol and phosphorous acid) were identified. With these data, estimates of the acute ecotoxicity values (solution toxicity values) based on the sum of the ratios of the maximum theoretical concentration of the individual hydrolysis by-products (i.e., "aged" TPPi) in solution (at the limit of solubility) and their representative ecotoxicity values (EC_{50}) were found to be 2.2×10^{-3} (algae), 2.7×10^{-2} (daphnids) and 3.1×10^{-2} (fish). Since a derived solution toxicity value of 1.0 is considered to be equivalent to an EC_{50} for the "aged" solutions, the further below a value is from 1 the lower the inferred ecotoxicity

hazard. On this basis, these findings indicate that the mixture of hydrolysis by-products arising from a standard solution of TPPi would not be toxic to aquatic organisms.

It is possible to quantitatively predict the maximum theoretical concentration of hydrolysis by-products and resulting toxicity of the solution of these by-product based on the known toxicity of the individual by-products, assuming additive toxicity.

On this basis, a detailed literature search was conducted to assess the available database of information pertaining to the acute toxicity of phenol and phosphorous acid to fish (rainbow trout), daphnids and algae. Where sufficient data were unavailable in the scientific literature, ECOSAR (US EPA 2001) was used to model the potential ecotoxicity of the hydrolysis by-products of TPPi. A summary of the acute ecotoxicity data for these byproducts to these organisms is provided in the report.

By this method, a solution toxicity value of 1.0 is considered equivalent to an acute EC₅₀ value (*i.e.*, it would predict 50% acute mortality /growth inhibition in the test species, based on the theoretical concentrations).

Results

Based on the following stoichiometry:

one mole TPPi (mw= 310.29 g/mole) yields three moles phenol (mw = 94.11 g/mole) and one mole phosphorous acid (mw= 82.00 g/mole);

At its aqueous solubility limit of 0.3 mg/L, TPPi would hydrolyse to 2.9×10^{-6} moles/L phenol and 9.7×10^{-7} moles/L phosphorous acid. These molar concentrations equate to mass concentrations of 0.27 mg phenol/L and 0.079 mg phosphorous acid/L respectively.

The modeling results of the solution toxicity values for the mixture of hydrolysis by-products of TPPi at its aqueous solubility limit in fish, daphnids and algae are summarized below.

Phosphorous acid, triphenyl ester (TPPi), CAS No. 101-02-0

Table 1: Aquatic Toxicity Values for the Hydrolysis By-Products of TPPi⁴

| Aquatic Toxicity Values | Phenol EC ₅₀ (mg/L) ^m | Calculated Phenol Solution Concentration (mg/L) | Phosphorous Acid EC ₅₀ (mg/L) ^c | Calculated Phosphorous Acid Solution Concentration (mg/L) | Calculated Solution Toxicity Value |
|-------------------------|---|---|---|---|------------------------------------|
| Fish | 8.9 | 0.27 | 383 | 0.079 | 0.031 |
| Daphnids | 10.1 | 0.27 | 387 | 0.079 | 0.027 |
| Algae | 144.2 | 0.27 | 230 | 0.079 | 0.0022 |

^m = measured value (derived from toxicity database, scientific literature).

^c = calculated value (using ECOSAR; US EPA, 2001).

Conclusions

The predicted solution toxicity values attributable to the mixture of TPPi hydrolysis by-products were calculated to be 2.2×10^{-3} (algae), 2.7×10^{-2} (daphnids) and 3.1×10^{-2} (fish). These values are well below 1.0 indicating that the mixture of hydrolysis by-products arising from a saturated solution of TPPi would essentially be not toxic to aquatic organisms. (Author)

Reliability

Klimisch Code: 2

References

GlobalTox International Consultants Inc., Guelph ON. "Consolidated Report - Alternative to Ecotoxicity Testing - Modeling the Potential Toxicity to Aquatic Organisms - Hydrolysis By-Products of Triphenyl Phosphite (TPPi) (CASRN 101-02-0)." Report to General Electric Company. July 29, 2003

HEALTH ELEMENTS

COMBINED REPEAT DOSE/REPRODUCTIVE/DEVELOPMENTAL TOXICITY

Test Substance

Identity: TPPi
Remarks: Doverphos 10, Batch 237T03101
Purity: 99.7%

Method

Method: OECD 422 (modified)

Phosphorous acid, triphenyl ester (TPPi), CAS No. 101-02-0

| | |
|--|---------------------------|
| Type: | 2 generation |
| GLP: | Yes |
| Year: | 2005 |
| Species: | rat |
| Strain: | Sprague-Dawley |
| Route of administration: | gavage |
| Doses/concentration levels: | 0, 5, 15 and 40 mg/kg/day |
| Sex: | Male and Female |
| Control group: | Yes, male and female. |
| Frequency of treatment: | once per day |
| Duration of test: | 16 weeks |
| Premating exposure period for males (P and F1) as appropriate: | 2 weeks |
| Premating exposure period for females (P and F1) as appropriate: | 2 weeks |

This study evaluated the potential of Triphenyl phosphite (TPPi, CAS No. 101-02-0) administered by oral gavage one daily, 7 days per week in CD rats, to cause toxic characteristics from repeated dosing, encompassing 2-week prebreed, mating (for both sexes), gestation and lactation (for F0 females) for F0 parents and direct dosing to F1 offspring from weaning to scheduled sacrifice at least 7 weeks post weaning. This study also evaluated the potential of TPPi to cause possible effects on parental male and female reproductive performance (such as gonadal function, mating behavior, conception, development of the conceptus, parturition) and offspring survival, growth, development through lactation, weaning, and through reproductive development until adulthood. This protocol exceeded the OECD 422 study design by following the F1 offspring to adulthood, with continued exposure and assessments of neurologic, immunologic and reproductive structures and functions. The protocol also assessed F0 recovery males, 28-day females and 28-day recovery females.

Male and female CD (SD) F0 rats were administered TPPi orally by gavage at 0, 5, 15 and 40 mg/kg/day at a dose volume of 5 ml/kg/day in Mazola[®] corn oil, 10 animals/sex/dose for 2 weeks of prebreed exposure (males and females), 2 weeks of mating (males and females), and 3 weeks of gestation and lactation each (F0 females) for F0 parents, and direct dosing of selected F1 offspring from weaning through scheduled sacrifice, at least 7 weeks post weaning. Five additional F0 males per group from the control and 40 mg/kg/day groups were designated as recovery animals and held without dosing for 2 weeks after the F0 male dosing period was completed, to evaluate recovery from any possible treatment-related effects identified in the high-dose group. Additional 28-day females (5/group at 0 and 40 mg/kg/day) and 28-day recovery females (5/group at 0 and 40 mg/kg/day) were also similarly assessed. Body weights and feed consumption for the F0 males and females were recorded weekly during the prebreed period, for F0 females during gestation and lactation, and for selected F1 offspring from weaning through scheduled sacrifice. Clinical signs were recorded at least once daily for F0 males and females and F1 offspring. Functional Observational Battery (FOB) including

home cage observations, handling observations, was performed on all initial animals once during quarantine and at least once per week for F0 animals during prebreed, mating (both sexes), gestation and lactation (F0 females) treatment periods and on 5 F1 females and 5 F1 males once midway during the post wean exposure period. After the 2-week prebreed exposure period, animals were randomly mated within treatment groups for a 2-week mating period to produce the F1 generation, with continuing exposure. Five each of F0 males and females per dose group were evaluated for auditory function, motor activity, and assessment of grip strength prior to necropsy. Grip strength was also assessed for the 5 F1 males and F1 females per group selected for FOB during the last week of the post weaning exposure period.

All F0 parental animals, non-selected F1 weanlings and retained F1 adults were necropsied with complete histologic evaluation of 5 selected F0 males and females in the 0 and 40 mg/kg/day groups. Because of extreme toxicity in the F1 offspring at 40 mg/kg/day, no F1 offspring were retained after weaning. Therefore, tissues from 5 F1 males and females per group at 0 and 15 mg/kg/day were examined histopathologically.

On the day of birth (postnatal day [pnd] 0), anogenital distance was measured and body weights recorded for all live F1 pups in all litters. F1 litters were culled on pnd 4 to yield as nearly as possible, 5 males and 5 females per litter. The culled F1 pups were weighed, euthanized, and necropsied with complete external and visceral examinations. For the remaining F1 pups, survival indices were calculated at least weekly through weaning (pnd 21). At weaning, at least 1 female and 1 male (whenever possible) from each F1 litter at 0, 5 and 15 mg/kg/day were randomly selected for a total of 10/sex/group to continue treatment for approximately 7 more weeks, with dosing for F1 selected pups begun on pnd 22 until all pups were at least 70 days of age. F1 post weaning observations and procedures for each retained F1 female included examination for vaginal patency (VP, from pnd 22 until acquisition of vaginal opening) and determination of estrous cyclicity and normality evaluated by vaginal smears taken daily the last 3 weeks of the post wean exposure period prior to scheduled sacrifice. For each retained F1 male offspring, observations for cleavage of the balanopreputial (preputial separation, PPS) began at 35 days of age and continued until acquisition of PPS. Andrologic assessments were also performed on the F1 retained males at necropsy. Histopathology was performed on F1 males and females (5/sex/group) at 0 and 15 mg/kg/day. In addition, hematology, clinical biochemistry and urinalysis (males only) were performed at necropsy for 5 randomly selected parental F0 males and females and for F1 adult males and females per dose group.

Results

TPPi administered by gavage once daily at 0, 5, 15 and 40 mg/kg/day to parental F0 CD (SD) rats, 10/sex/group, through prebreed, mating and gestation and

lactation and direct dosing to the F1 offspring (10/sex/group) from weaning to scheduled sacrifice, resulted in adult F0 parental toxicity at 40 mg/kg/day, increasing over time (reduced body weights, ataxia, and foot splay). Reproductive toxicity was not present in F0 males or females. There was profound F1 offspring toxicity observed postnatally during lactation at 40 mg/kg/day (so the group was terminated on pnd 21) , including increased mortality, especially for pnd 0-4 and reduced pup body weights/litter starting on pnd 7-21. Acquisition of puberty in F1 males and females was unaffected. Twenty eight-day males (same as F0) and females and 28 day recovery males and females exhibited the same progressive systemic toxicity at 40 mg/kg/day as in the F0 parental animals, although the effects were less severe, most likely due to the shorter dosing duration.

Conclusions

The F0 male and female systemic no observable adverse effect (NOAEL) was 15 mg/kg/day. The NOAELs for F0 reproductive toxicity were at or above 40 mg/kg/day for males and females. The NOAELs for F1 offspring toxicity during lactation were 15 mg/kg/day for males and females. The F1 male and female systemic NOAEL was also 15 mg/kg/day.

Reliability

| | |
|----------------|---|
| Klimisch Code: | 1 (Reliable without restriction) |
| Remarks : | This study was performed under OECD (1998) and EPA TSCA (1989) Good Laboratory Practice regulations. (Author) |

References

Tyl, RW, Myers, CB and Marr, MC. "Modified Combined Repeated Dose Toxicity Study with the Reproductive/Developmental Toxicity Screening Test of Triphenyl Phosphite (TPPi; CAS No. 101-02-0) Administered Via Oral Gavage to CD® (Sprague-Dawley) Rats (OECD 422)." RTI Identification No. 65C-09165.000.400. Report to Crompton Corporation, RTI International, Research Triangle Park, NC. November 12, 2004.